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MICROSTRUCTURE–PROPERTY–DESIGN RELATIONSHIPS IN THE SIMULATION ERA: AN INTRODUCTION (PREPRINT)

Dennis M. Dimiduk

Metals Branch
Metals, Ceramics & NDE Division

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MATERIALS AND MANUFACTURING DIRECTORATE
WRIGHT-PATTERSON AIR FORCE BASE, OH 45433-7750
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Computational methods are affecting a paradigm change for using microstructure–property relationships within materials and structures engineering. This chapter examines the emergent use of quantitative computational tools for microstructure–property–design relationships, primarily for structural alloys. Three major phases are described as a historical 'serial paradigm,' current 'integrated computational materials engineering' and, future 'virtual materials systems' emerging from advances in multiscale materials modeling. The latter two phases bring unique demands for integrating microstructure representations, constitutive descriptions, numerical codes and experimental methods. Importantly, these approaches are forcing a fundamental restructuring of materials data for structural engineering wherein data centers on a hierarchy of model parameterizations and validations, rather than the current application-specific design limits. Examining aspects of current research on microstructure-sensitive design tools for single-crystal turbine blades provides an accessible glimpse into future computational tools and their data requirements.

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Microstructure–Property–Design Relationships in the Simulation Era: An Introduction

Dennis M Dimiduk

Abstract

Computational methods are affecting a paradigm change for using microstructure–property relationships within materials and structures engineering. This chapter examines the emergent use of quantitative computational tools for microstructure–property–design relationships, primarily for structural alloys. Three major phases are described as a historical 'serial paradigm,' current 'integrated computational materials engineering' and, future 'virtual materials systems' emerging from advances in multiscale materials modeling. The latter two phases bring unique demands for integrating microstructure representations, constitutive descriptions, numerical codes and experimental methods. Importantly, these approaches are forcing a fundamental restructuring of materials data for structural engineering wherein data centers on a hierarchy of model parameterizations and validations, rather than the current application-specific design limits. Examining aspects of current research on microstructure-sensitive design tools for single-crystal turbine blades provides an accessible glimpse into future computational tools and their data requirements. Finally, brief descriptions set context and interrelationships for the remaining chapters of the book.

1 Microstructure–Property–Design Relationships & Structural Materials Engineering

Present-day advancements in microstructure–property relationships are coming about via computational methods. The efforts largely recognize that microstructure–property relationships evolve over a wide range of scales and that both technical and computational advances must occur for adequate representations of these relationships within predictive tools. However, many of these efforts fall short of full recognition that engineered materials are systems. What is needed is a computational methodology and framework for systems engineering of materials and the sciences

that support such an approach. The systems engineering of materials within a simulation environment will provide advances to both materials utilization and the representations for usefully advancing quantitative microstructure–property relationships. To better understand what is needed from the computational framework, it is useful to briefly examine materials in present-day engineering.

About 100 years ago, a defining aspect of materials science and engineering (MSE) had its origin in the first microscopy studies of materials structure; yet, nearly a half-century would pass before their impact evolved into the MSE discipline (Smith 1988, Cahn 2001, Olson 1997). With the study of microstructure (including defect structure), the materials engineer gained an important tool by which processes and properties are controlled. Microstructure–properties science was born and has expanded ever since. Materials science and engineering now recognizes four major disciplines of practice that identify the unique character of the MSE field: processing–structure–properties–design, irrespective of the material type, class or design application (see Figure 1). However, unlike other mainstream engineering disciplines (civil, chemical, electrical & mechanical for example) that largely came into existence as the quantitative frameworks for them emerged, the same cannot be said for MSE.

More broadly speaking, structural alloys tend to be defined from two different perspectives. Materials producers (and patent law) associate them with compositions of matter and the prescribed synthesis and process paths by which they are formed into engineered products. Alternatively, from a structures-design engineering perspective, materials are viewed as contextual databases containing representative measured values of property bounds, including statistical minima, as functions of selected variables such a temperature or state of stress. These are often represented within models. The contextual aspect of those databases often relates to specific application products and manufacturing processes. Additionally, the structures engineer also attributes the businesses and practices that make materials available as products to the materials engineering discipline. Historically, the metallurgist, ceramist or chemical engineer and, more recently the materials-scientist or engineer, carried out the onerous task of melding these perspectives into unified activities and practices for safe and affordable structures. Within this engineering reality, the notion of microstructure–property relationships is only implicit at best. While both materials and process engineers and part designers recognize that structural materials have significant microstructural variations, there are few quantitative tools and standards that permit integration of that knowledge into the broad engineering process, especially in a predictive manner. Consequently, outside of the MSE community, processing–properties–design relationships (not including structure) are generally recognized via the “allowables” for using a material for a given design.

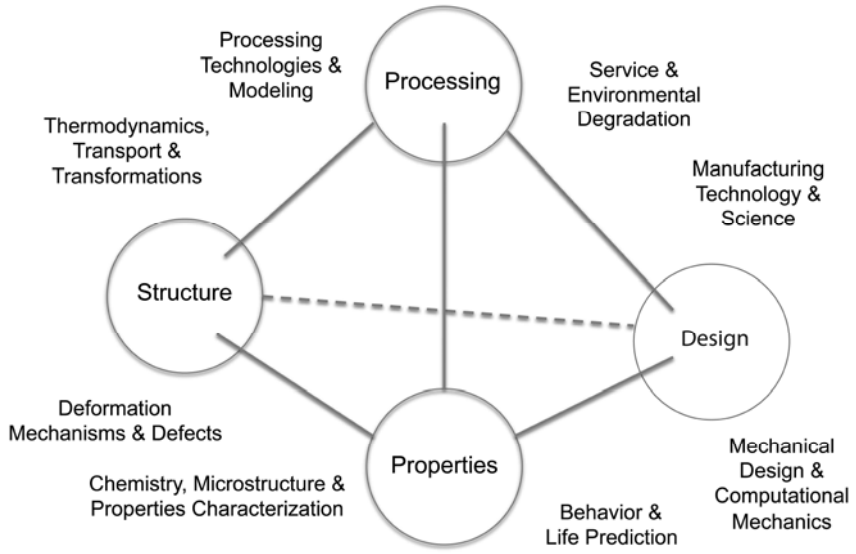

Figure 1: The four defining disciplines of practice for materials science and engineering (MSE) represented as a tetrahedron. In this context "Processing" refers to composition, synthesis and processing in general. "Structure" refers to all aspects of microstructure, including both intrinsic and extrinsic defects from the atomic to macroscopic scales. "Properties" and "Design" refer to materials performance and behavior and, to engineering design rather than materials design, respectively. Selected examples of the types of studies and activities that tend to link the major disciplines are shown about the periphery of the figure.

For most of today's products, one typically defines an application and then seeks to define and document a processing specification through specific suppliers by which a selected composition of matter will reproducibly lead to properties (performance) for that application. Material microstructure descriptors, such as grain size (ASTM 2004), are only used as specifications of the material for process assurance. For higher value engineered structures (e.g. a gas turbine engine disk), a database of processing–properties relationships typically develops in which the data are reduced to phenomenological constitutive laws that are linked to the application design process via finite element method simulations of the part configuration. With few exceptions, these constitutive relationships are assumed to hold over volumes of material that are essentially on the scale of the part (meter scale), even though every metallurgist or

materials scientist understands that heterogeneities or defects that affect properties exist over many length scales from the full part to the atomic level. Clearly, there is a disconnection between MSE, and the broader engineering community as the notion of processing–structure–properties–design essentially does not exist beyond MSE.

This disconnection is a rational result of the fact that even after a century of development the quantitative links between processes and structure and, structure and properties, are insufficiently advanced to permit direct systems-oriented optimization of materials and products (McDowell and Backman Chapter 17). There is simply too much complexity associated with the kinetics of processes to quantitatively define the resulting microstructures within the equally complex hierarchy of length and timescales of the applications. For electronic materials the length and timescales may be extremely small fractions of seconds and nanometer dimensions, while for structural composites they may be at the scale of the components and system dimensions (meters) over timeframes of years.

Fortunately, current advances in computing capabilities and MSE tools bring opportunities for not only expanding the quantitative basis for processing–structure–property–design relationships within simulation environments; but also, an opportunity for redefining aspects of MSE within those simulation environments. In so doing MSE becomes a quantitative engineering discipline for structural materials and several aspects of its relationship to other engineering disciplines will be redefined. Full recognition of this opportunity stems from considering aspects of the use of computer modeling and simulations along the evolutionary path of MSE.

2 Computational Materials Science for Microstructure

Computers and simulation were available essentially since the origins of MSE as a recognized discipline. Several phases of their use in MSE are linked to growth in computational capacity and databases. In the 1950's and 1960's, the computer was commonly used to model specific phenomena, usually within a mean-field, especially where numerical solutions to differential equations were necessary. From a materials engineering perspective, perhaps the best example of this is the computer calculation of phase diagrams or the "CalPhad" method that was well developed by the end of the 1960's (Kaufman and Bernstein 1970). During that period foundations were built for materials-oriented computer simulations that last to this day (see additional diverse examples such as computing diffraction contrast of transmission electron microscopy images (Head et al. 1973) and plasticity analysis for metal deformation (Mandel 1973, Kocks 1987) to name but two others. Importantly, even though the foundational sciences were known more than forty years ago, neither the computational capacity

nor the necessary data bases were sufficiently developed for the CalPhad method to have significant engineering impact at that time for alloy or process development. Only about ten years ago did the method begin to add value to engineered products and the practices of MSE. Today, after more than a decade of sustained development investments for engineering, CalPhad techniques are becoming a part of standard industrial methods (NMAB 2008, Backman et al. 2006).

A second phase in the maturation of materials computational methods occurred during the 1970's and 1980's through research in process modeling. Simulation codes evolved that are still in use today (ProCAST http, DEFORM http). These codes, based on continuum fields and state variables without treatments of microstructure, are essential to design engineering of high-value-added aerospace components. Also during this period, methods for solving a range of materials challenges from the electronic structure of materials to techniques for plasticity and stress analysis continued to advance (Hafner 2000, McDowell 2000). Methods for simulating plasticity under crystallographic constraint within the finite-element method gave new insights into behavior at the mesoscopic scale (Asaro 1983).

One could say that during the late 1970's through mid 1980's, computational materials science (CMS) came into its own as a discipline of study. Here, the term CMS refers to the activities of a widespread community of investigators that are developing simulation tools to represent unit mechanisms exhibited by materials. These include such techniques as electronic structure methods for selected material properties and thermodynamic quantities (Hafner 2000, van de Walle 2002, Liu 2006); empirical atomistic methods that offer insight into understanding dislocation core structures, surfaces and grain boundaries (Daw and Baskes 1984, Vitek 1985, Tschopp et al. 2008); dislocation dynamics methods (Devincre et al. 2001, Ghoniem et al. 2000); phase field methods and, many others. A good compendium of such methods may be found in the work edited by Yip (2005).

However, the majority of the CMS-based advances in understanding mechanisms of materials behavior had little or no impact on materials engineering. While the quantitative nature of simulated results improved, too frequently they lacked comprehensive context or sufficient accuracy for use in engineering design. The few applications of simulation-based results to real-world microstructure–properties engineering tended to use simulation results to provide qualitative insight into existing engineering processes (see for example Dimiduk 1998); however, there were notable exceptions (Shercliff and Ashby 1990). There are numerous reasons for this, but obvious among them was insufficient computational capacity together with the integrated data available during that time.

Throughout the 1980's and 1990's, much of the materials simulation efforts were performed in relative isolation within the MSE, physics, mechanics and chemistry communities largely without any linkages to engineering techniques or design tools.

Unlike other engineering disciplines, the role of simulations within MSE continued to be viewed to a great extent as only interesting or important for understanding qualitative behavior trends. Throughout this period, there were few efforts outside of the process-modeling discipline that attempted to integrate mechanistic or heuristic knowledge within simulations to understand the microstructure–property relationships in engineered products. Although some researchers recognized that the quantitative aspects of microstructure–property relationships were underdeveloped (Cedar 2000), CMS was often characterized as simply "applied quantum mechanics" (Bernholc 1999). During this period, CMS was essentially a 'cottage industry' of models and modelers of and to itself (Dimiduk et al. 2004b).

During the mid and late 1990's, a few industry, government and academic leaders began to see the limiting aspects of this view of CMS (see for example Olson 1997, Christodoulou DARPA-AIM http, Fraser CAMM http). These leaders recognized that CMS approaches to materials modeling typically originated from the 'bottom up' of the length and time scales and that such approaches rarely made an impact on the practices or efficiencies of design engineering, especially for structural materials. Further, there was recognition in the MSE community that significant computing capability was becoming sufficiently widespread that new approaches to simulation-based materials engineering should be attempted from the 'top down'. As a result two notable new initiatives in computational-based materials engineering were initiated in the first year of the new millennium (NMAB 2008).

3 Integrated Computational Materials Engineering

3.1 Materials Readiness and the Evolving Microstructure–Properties–Design Paradigm

To best understand the uniqueness of the integrated computational materials engineering (ICME) approach and its impact on the practices associated with microstructure–properties–design relationships, it is useful to first understand the concepts of materials engineering readiness. Materials development and process engineering involves significant open-ended risk and cost. To manage and mitigate that risk, the MSE community adopted various frameworks for assessing readiness along the pathway toward product application. These frameworks are similar to ones used for other engineering but are tailored (especially within major manufacturing companies) to materials and processes disciplines. Figure 2 illustrates the highest-

level structured ‘stage-gate’ process that exists within most materials and processes practice. Typically, ten levels of readiness are defined and the progression of application-specific technologies through these levels occurs within well-defined engineering templates. These templates demand specific test data, cost assessments, manufacturing source qualification, etc. that gain fidelity *and scope* at each stage of development. This serially staged paradigm of materials and processes technology maturity, to some degree reflects the learning curve that innately exists for anything new. Unfortunately, the expanding scope required at each step is a key limiter to this paradigm that adds significant risk and quite often cost.

Reviews of case studies of materials development that follow a serial paradigm have shown that it leads to serious challenges for materials development and limits the opportunities for coupling materials and process advancements within mainstream engineering design practice (NMAB 2008, NMAB 2004, Lipsitt et al. 2001, Dimiduk 2001, Dimiduk et al. 2003). The serial paradigm leads to what has been called the “valley-of-death” for new materials and processes. That valley exists for several reasons including funding gaps, long time requirements for experimental or empirical iterations and, what may loosely be called a ‘point contact’ interface between present-day design engineering and materials engineering.

To further illustrate this, Figure 3 schematically depicts the broad engineering procedural steps that may be used to select the geometric configuration of a manufactured aerospace metal component. The figure also shows selected materials and processes procedural steps that are taken to assure appropriate microstructure–property relationships are maintained in the final product. Inspection of the figure reveals that the primary interface between the design process and the materials development process lies in the steps needed to assure that validated constitutive descriptions (or minima curves and allowables) are available for the design optimization procedures. Thus, within this schematic depiction, the interface between the communities is a point contact. This point of contact includes not only the constitutive laws that reside within component design codes, but also their empirical validation against databases that must sufficiently encompass the variations of microstructure–property relationships judged to be important to the specific design. Given that the allowables databases are produced from application-specific, full-scale development hardware, this serial approach inevitably leads to a conservative estimation of material performance and does so via a costly process. Since part-specific and feature-specific microstructures and properties cannot be accounted for

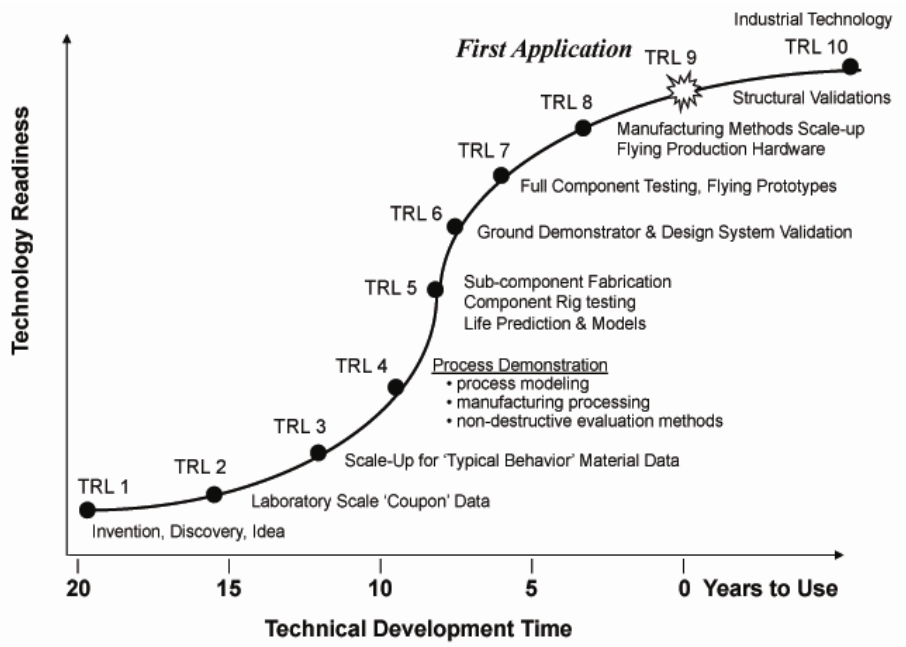

Figure 2: General technology readiness levels (TRL) for materials. The 10 stages of materials readiness are adopted from the broader engineering readiness metrics used for products and systems. Historically, achieving the transition from TRL 3 to TRL 5 is the most difficult step. The reason for this is that technical risks typically remain high at TRL 3; however, the financial outlays required to mitigate them also grow much more substantially at this stage by comparison to the lower levels. Better materials and processes simulation tools are needed throughout, but especially for risk mitigation through the TRL 3 to 5 maturity levels. For aerospace materials, evolutionary advances (such as modified alloy compositions within established applications) are known to require 7-12 years to reach first use. For more challenging completely new materials, such introducing ceramic composites or TiAl alloys in turbine engines, the time span for achieving fist-use readiness exceeded 26 and 36 years, respectively.

within the design system, the observed “worst-case” uncertainties are assigned to all parts at all locations (Christodoulou and Larsen 2004). Consequently, microstructure–property relationships are specified and controlled in the context of their application

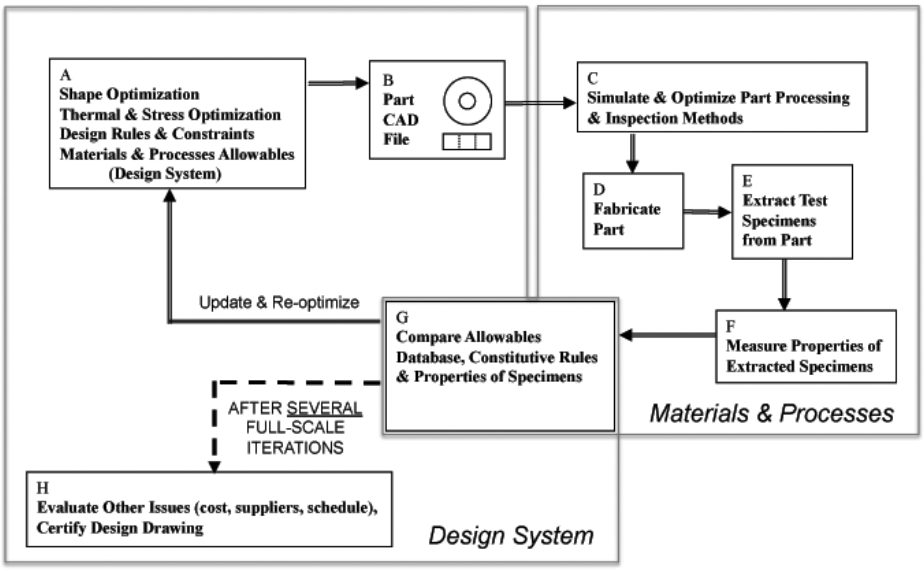

Figure 3: Schematic representation of activities within of today's experiment-intensive processing–properties–design serial paradigm for materials engineering. The methodology has no explicit consideration of microstructure. Microstructural effects are only implicitly considered when extracting specimens and as selected specifications for parts. Microstructural effects/variation is represented through expensive, time-consuming testing and multiple full-scale process and test iterations are usually required.

databases alone, usually via testing of full-scale prototype parts. However, further advancement in the design process demands a less conservative and more realistic, probabilistic approach (McClung et al. 2008, Millwater and Osborn 2006). That new demand is driving the MSE community toward developing predictive tools for location-specific properties that can be used within probabilistic design tools.

Herein lies one major hurdle for microstructure–properties sciences and materials development in general. As long as materials behavior can only be indirectly defined within the very specific contexts of their applications, via extensive testing of samples excised from full-scale prototypes that may not even directly capture the design features of interest, materials development will always entail long development times and high costs. That fundamental limitation in the procedure for obtaining and representing materials performance data presently place the whole of MSE into a unique domain that is outside of those of the other engineering disciplines. The time

scales, cost structures and design tools are simply mismatched, while the risk is high. Today one develops empirical knowledge of materials response to chemistry and process iterations within the stage-gated templates described previously, such that learned practitioners of the engineering disciplines can support design judgments. Those judgments inevitably entail reasonable assurances to business managers that the financial investments in scale-up and advances in technology readiness are affordable within business plans and product timing. For the future, materials development needs to be achieved via a new materials-to-design paradigm. Essential to that paradigm is that the materials readiness structure (readiness templates) be re-cast to maximize the scope of readiness information at the earliest stages; then, to expand only their fidelity with added development investments and time. Fortunately, efforts toward building these are well underway.

3.2 Accelerated Insertion of Materials, Virtual Aluminum Castings and the ICME Paradigm

Today the computational tools that facilitate quantitative support for the development and investment judgments required for materials scale-up are just emerging. Examples of these exist within the ICME demonstration efforts that occurred during this decade (NMAB 2008). Essentially, the underlying concept behind the efforts is that having simulation tools for all aspects of new product and materials development will reduce development time while lowering costs and risks. Two notable examples of the ICME paradigm will now be discussed.

Within the aerospace sector, the Accelerated Insertion of Materials (AIM) program was sponsored by the US Defense Advanced Research Projects Agency (DARPA) and the United States Air Force, to examine and restructure the paradigms for metal and organic-composite materials development (NMAB 2008, Backman 2006, Dimiduk et al. 2003, Dimiduk et al., 2004). Similarly, within the automotive sector the Virtual Aluminum Castings (VAC) program, was sponsored by Ford Motor Company (NMAB 2008, Allison 2006). In the specific sense of microstructure–property relationships, the efforts showed that representing the microstructural aspects of materials (especially including kinetic and mechanical behavior), via models that function within design-engineering optimization software, yields dividends to the product development cycle. Importantly, the case studies showed that even elementary theory and empirical models have a substantial positive impact on the design engineering process when employed within a computational environment (NMAB 2008, Dimiduk et al 2003). Somehow, that important payoff to engineering

was missed by most of the CMS and MSE communities. Also, when viewed from the perspectives of these demonstrations, there is now a clear justification for expanding the fidelity of microstructure–property representations and predictive capabilities and, also a somewhat general template for both focusing those developments and then integrating them into the product value stream as they occur.

The materials and processes development paradigm has changed with the evolution of ICME. Figure 4 shows a similar schematic as the one previously described in Figure 3, but with modifications that reflect broad procedural changes brought about via the ICME approach as it was applied in the AIM program. Two aspects of the new procedure are noteworthy. First, as shown by the expanded activities associated with step "C2" (in the upper right-hand side of the figure), specific simulation tools focused on microstructure–property relationships enter into the development paradigm. Second, utilizing such tools fundamentally changes the experimental activity that currently takes place to empirically assure the manufactured products perform in the desired fashion. Rather than many full-scale synthesis and processing trials followed by sectioning and testing, many of the results of such efforts are now anticipated via simulations. Having models, even in empirical form, integrated with the design process permits iteration and optimization via design tools and minimizes the time-consuming and expensive procedures associated with full-scale prototype product development. Thus, the overlap between engineering design and MSE fields of practice has expanded. That expansion is the direct result of using simulation tools to provide a more quantitative and structured description of the microstructure–property relationships of materials. A widespread acceptance by a peer group of engineers, systematic reductions in the types, cost and quantity of data needed and, the predictive nature or capabilities of the microstructure–properties relationship tools used within such a paradigm, are all direct measures of the quantitative advance of the field. Future advances in computational methods for microstructure–property relationships should be evaluated by those metrics.

3.3 The Evolving Needs for Materials Data

Another important aspect of the ICME paradigm for materials not explicitly shown in Figure 4 was a significant aspect of the both AIM and VAC feasibility demonstrations. That aspect pertained to the development of models and the nature of experimental data. Within the historical processing–properties–design paradigm for materials critical design data exists almost entirely in the form of measured mechanical proper-

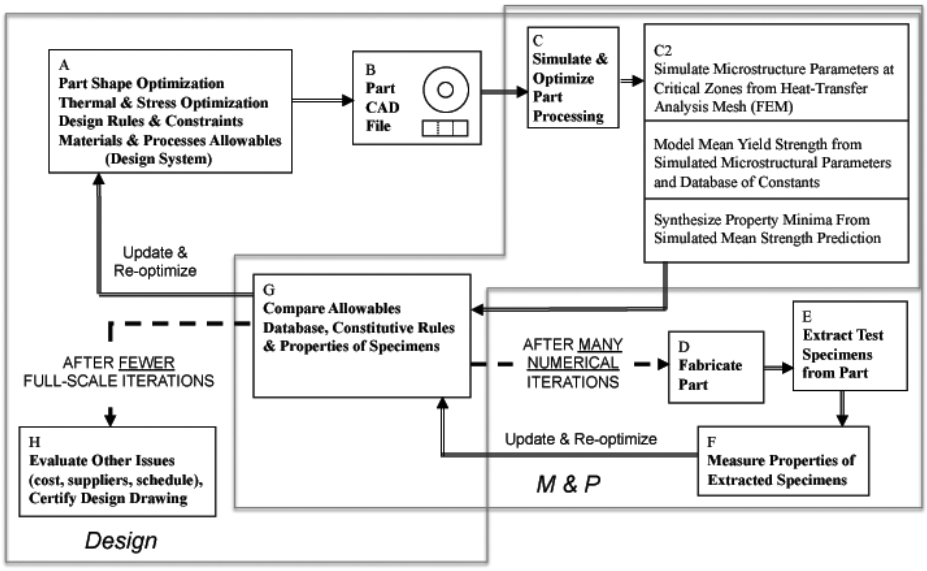

Figure 4: Schematic representation of activities within ICME paradigm for materials engineering (see text for explanation). Methodology explicitly includes microstructural-based design via microstructure evolution within process models and, mechanical property models being applied to various regions of designed part. Including microstructure–property relationships via simulations means that the domains of design and materials engineering overlap much more significantly within ICME than within the historical paradigm for materials engineering. The ICME paradigm includes the first cases of explicitly using processing–structure–properties–design within closed-loop engineering frameworks.

ties obtained from production-scale hardware—again, having little explicit tie-in to microstructure. However, the ICME paradigm changes the structure and types of data that are essential to design. *Under the ICME approach, data must be associated with models and supported simulation codes*. Also, specific types of data are collected for the primary purpose of validating codes. That data often extends outside of the ranges typically associated with prototype parts and may be associated with certain pedigree-type materials and microstructures. Fortunately, as simulation tools and models become more advanced test and evaluation procedures have become automated and

miniaturized. Critical data can increasingly be measured from small-scale samples prepared to validate kinetic or mechanical behavior domains for models.

The last paragraph discusses points that are non-trivial and merit further comment. For example, the nature of data intrinsic to an expanding ICME paradigm is data associated with simulation tools and their validation. Those tools by their inherent architectures and operative material models define the data required for their use. In this respect, the ICME paradigm is in its infancy and aspects of data taxonomy and efficiencies must be developed for the purposes of supporting simulations. However, even from the initial case studies just described, the ICME paradigm suggests a different view of data and materials informatics than the one described by recent reports on the subject (Cebon and Ashby 2006, Arnold 2006). Those reports essentially describe higher-fidelity extensions of the classical MSE-design paradigm—a paradigm constrained by the serial development of handbook materials allowables. Within that paradigm, the role of the computer is 'passive' in that it primarily facilitates the organization of greater quantities of information. When data sets are sufficiently large and too complex for typical human interrogation, this paradigm may facilitate the 'blind discovery' of new relational knowledge (data mining) in a more 'active' mode.

However, computational tools and simulation environments are beginning to synthesize data that may be fused with conventional empirical measurements (Liu et al. 2006, van de Walle et al. 2002). The practice is likely to spread far beyond its present use within alloy thermodynamics. Yet there is little readiness for this within the old processing–properties–design paradigm and the practice is limited even within the current ICME paradigm. The MSE and design communities have a formidable task ahead of them to define appropriate data architectures and a taxonomy that will not only permit full 'active' utilization of materials simulations in the design process but also maintain efficient certifiable engineering practices throughout the new simulation era. Within an emergent paradigm called "virtual materials systems" that taxonomy and the actual data are facets of the substantially expanded and quantitative nature of microstructure–property relationships. Finally, the new ICME paradigm suggests that the materials allowables view of data will change to more effectively utilize the active power of materials simulations for 'synthesizing' data and providing quantitative insights into materials response.

3.4 ICME: Lessons Learned

There is value to considering lessons learned from the initial case studies of AIM and VAC. The recent report by the US National Materials Advisory Board discusses some

of these lessons (NMAB 2008), but a selected three global aspects are highlighted here. First, for the longer term, the contrasting primary attributes of engineering design and MSE must be bridged. For engineering design, those attributes include a simulation-centric community of practitioners, education structures that convey such practices, well developed and supported simulation tools that are integrated with heuristic data and, the expectation that many rapid-time-frame simulations will be carried out as a routine part of the design process. Conversely, the primary attributes of MSE in this regard currently include long lead times for experiment results within a data focused community of practitioners, an educational system that is just now grappling with an appropriate treatment of ICME and its tools, relatively few established and supported simulation codes that are still too separated from heuristic data and, a general expectation that when simulations are done they will commonly be characterized by relatively few large-scale simulations performed in a supercomputing environment. As aspect of the previous discussion and portions of this book support, the gap between these communities exists in no small part because of the still under-developed quantitative sciences associated with materials microstructure–properties kinetics and mechanical behavior.

A second lesson contained in ICME is that the engineering design paradigm needs to evolve to explicitly include material heterogeneity within engineered parts (read microstructure–property–design relationships). In present day design practice, those aspects of heterogeneity not broadly included in databases or represented in analytical and simulation tools tend to be captured via heuristic rules that constrain the design process. For example, heterogeneities within materials lead to a variation in the performance for identically designed parts and populations of those parts perform differently. Consequently, that variability in parts often leads to the costly replacements of part populations based upon time in service, rather than conditional replacement tied to specific part behavior (Christodoulou and Larsen 2004). In the longer term the development of simulation tools must strive to mitigate the need for heuristic rules by integrating sensor measurements of the service history and environment into materials response models. In that way the design and user communities would also gain tools to assess variations in the structural part life that result from variations in their application environments. Conversely, it is important for the ICME and CMS communities of practice to recognize that in most cases of engineering design, there is an incomplete understanding of details of the use or operational environment even with sensor measurements. Thus heuristic rules will always be a part of the design system to varying degrees and both design and materials must strive for robustness.

A third key lesson focuses on the notion that all engineering design proceeds from “representations” of the desired properties, behavior phenomena, part-geometry, design constraints and, the materials from which parts are constructed. The materials

engineer should ask of every item of interest "how should this item be modeled and represented in the optimization framework for design?" The whole of this book focuses on selected aspects of microstructure–property representations. However, engineering design demands representations for many additional aspects of the product value-stream that could interact effectively within simulation-based materials properties tools (McDowell and Backman Chapter 17). Thus, the nature of the representation used in simulation for a selected attribute or property is one clear measure of present-day understanding, relative importance and tractability of the attribute within the design and simulation environment.

The examples of ICME to date suggest that simulation-based approaches to microstructure–properties relationships can be effectively used in the design process to add value to engineered products. Thus, it is reasonable to expect that the fidelity of those tools for the representations of microstructure–property relationships will also grow. Consequently, it is useful to consider where the expansions of microstructure–property science may lead within the modeling and simulation era.

4 Multiscale Materials Modeling, Materials Systems Simulation Science and Virtual Materials Systems

Present-day advancements in microstructure–property relationships are coming about via the techniques of multiscale materials modeling, especially concurrent multiscale modeling. Those efforts largely recognize that microstructure–property relationships evolve over a wide range of scales and that advances must occur for adequate representations of these within predictive tools. However, even most of those efforts fall short of full recognition that engineered materials are systems. What is needed for MSE and CMS is a systems approach to materials simulations and the sciences that supports such an approach. The systems engineering of materials within a simulation environment will provide the usefully structured advances to both materials utilization and the tools for quantitatively representing microstructure–property relationships.

Given the context of materials engineering discussed previously, it is useful to peer into the future of microstructure–properties science and engineering. This book captures one view of that future via a selected look at a few of the advanced techniques in the field as well as some of the pacing state-of-the-art capabilities and challenges. The set of techniques is drawn from the editors' viewpoint that microstructure–properties relationships science is headed towards the development of "virtual materials systems" in every sense of the term. That is, just as the biological sciences are slowly evolving toward computer-based representations of systems (such as humans for example) that somewhat virtually function in the same ways as their

real-world counterparts, so too MSE should strive to supply computer-based systems representations of materials that mimic the real world behavior at all scales (Wikipedia Virtual Human http). This view of the future demands a full embrace of simulation tools as an integrating theme and, in some respects, a defining aspect of the quantitative microstructure–property sciences. The view also requires that research embrace the notion that materials rarely perform outside of a systems context (for example, a turbine engine airfoil system, or an automotive engine valve system, etc.).

4.1 Microstructure–Property Representation and Simulation

The engineering objective is to microstructure–property relationships together with engineered part designs within virtual materials systems. Quantitative predictions of part performance are obtained via numerous statistical instantiations of the material microstructure and the resultant simulated responses of those structures for a current part configuration. To achieve such simulation environments, one must recognize the fact that there are only four primary domains of freedom for simulations that collectively determine the quality and fidelity of the resultant predictions. Figure 5 depicts those domains for representing each aspect of materials microstructure–property relationships in a computational environment. Aspects of concurrent multiscale materials modeling strive to expand these four domains of materials representation by having the structure representation and perhaps even the constitutive description(s) evolve in an adaptive fashion as heterogeneities (such as local deformation or micro-cracking) evolve out of the initial representation. That simulation science involves quantitative management of error metrics, clear descriptions of failure criteria and, an intimate knowledge of the computing environment employed for the simulation set.

As depicted by Figure 5, there must be a multiscale representation of the structure and its microstructure that includes coarse-scale domains of the part, extrinsic defect structures, intrinsic microstructure, their statistics at various scales and, even the smallest-scale aspects that affect chemical kinetics. That representation must dovetail with the constitutive descriptions of the system energetics and evolution. For example, the constitutive descriptions may involve pseudopotential formulations for electronic interactions at one lower length-scale, empirical atomic interaction potentials at another scale, mean-field thermally-activated process models at a still larger scale, as well as the myriad mechanical behavior descriptions that are captured in present-day property models and design codes.

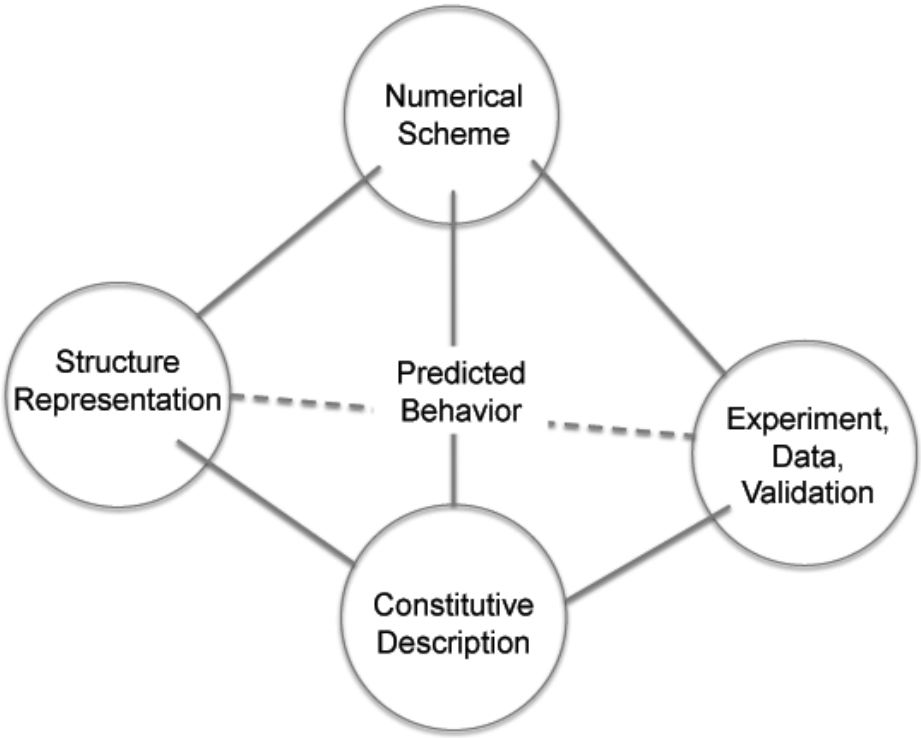

Figure 5: For any property of interest in design, there exists a multiscale hierarchy of microstructural effects that must be represented within simulation codes. However, as this figure depicts, within the computational environment there are only four broad domains of freedom for representing all of those aspects of the material. Recognition of these four domains provides a means for assigning each aspect of the material to the simulation environment and, by doing so, clearly identifies the coarse-graining inherent to the selected technique.

However, to select the most appropriate modeling and simulation development pathway it is not enough to know the constitutive relationships and structure representation alone; one must also know the context of the system, or design requirements that are to be simulated. Both of these in turn must align with all aspects of computational tractability of the simulation methods represented in the figure by the domain of numerical schemes. For example, today there is little ability to represent thermally activated processes within parametric dislocation dynamics simulations,

making the present form of that numerical environment a poor choice for studying the creep behavior of materials. Similarly, as some of the chapters in this book reflect, there is a growing ability to use explicit grain-level representations of microstructure within continuum constitutive descriptions of flow to examine deformation localization and instabilities for a variety of materials. However, going still further, as these explicit microstructural methods emerge so too must the constitutive descriptions evolve since the present ones tend to coarse-grain at an inappropriate scale. Evolving methods for concurrent multiscale simulations will eventually permit localization and time-dependent failure initiation when structure representations and constitutive rules are tailored for those methods of solution.

Finally, the aspects of the material that are not represented within the previously described domains of structure representation, constitutive laws or numerical schemes, must be brought to the simulation via measured quantities or empirical calibration parameters. Obviously, there should be recognition that experiments are as much a part of multiscale materials modeling as the simulations themselves. Consequently, there are new quantitative tools emerging for approaching those experimental challenges (Zhao 2006, Uchic et al. 2006, Rosenburger Chapter 16).

4.2 Single-Crystal Turbine Blades—An Emerging Case Study

The design and manufacture of turbine engine airfoils is a multibillion dollar-per-year industry. The materials and designs used for the single-crystal high-pressure turbine airfoils represent a limiting aspect of these ubiquitous engines. Since the efficiencies of the engines depend upon the maximum temperature of the gas path, there is a sustained need to find materials and designs that permit continued gains.

4.2.1 A Prototype Challenge

In recent years, the operating temperatures of turbine engines have risen to the melting point of the Ni-superalloy single-crystal materials used to make the hot section airfoils. Clever designs and manufacturing methods that permit cooling air to flow through the interior of the airfoil, coupled with complex zirconia-based coating systems on the exterior portions exposed to the combustion gases led to such high performance capabilities (Reed 2006). They have also resulted in complex states of time-dependent stress during service and are an interesting example of applications where dimensional constraints imposed by aero-thermal design interact with materials

at dimensional scales comparable to microstructural dimensions. The continued evolution of these highly engineered hybrid material systems demands advances in design methodology, which today resides principally with anisotropic elasticity and homogeneous descriptions of material response (Meric et al. 1991, Arakere and Swanson 2002, Harrison et al. 2004). What is needed for turbine blade design is a computationally tractable, higher-fidelity design system that permits a better analysis of the spatial-temporal stress state and damage accumulation in a representative environment.

Figure 6 shows that the aerodynamic and cooling geometry design features of cooled airfoils (wall thickness, cooling channels and ribs, etc.) are on the scale of the primary material microstructure. Thus, any variation of the material may lead to variations in airfoil behavior from region-to-region and from airfoil-to-airfoil, simply as a result of those variations occurring at differing locations relative to the designed geometric features. How does one best use computational methods, especially for microstructure–property relationships, to permit such assessments within the design process? How might an airfoil designer assess the probability of the weakest-link or life-limiting microstructural feature occurring at the geometric feature that most limits the design? To begin to answer these questions, one must examine not only the nature of the material microstructure–property relationships, but also their representation in design simulation codes, as previously suggested by Figure 5. One must devise representations of the material's structure and its response to time-dependent loading states, all within some context of numerical frameworks that may be used to perform design simulations.

Figure 6 also shows examples of microstructural variables that can be important to performance variations across a population of turbine airfoils of a constant design and manufacturing process. These arise from both the complexity of the superalloys themselves and the methods of their manufacture (Pollock and Tin 2006). Figures 6b-e, show examples of mis-oriented or low-angle grain boundaries, the dendritic microstructure that results from chemical segregation during casting solidification and, a mixture of eutectic microconstituent, carbides and pores, respectively. Freckle grains may lead to locally high stresses since these are local polycrystalline regions. The low angle boundaries are a generally accepted feature of the otherwise single-crystal materials; however, the superalloys exhibit severe crystal orientation sensitivity to their creep behavior (MacKay and Maier 1982). Thus, design should be able to assess the stress states relative to these features when the airfoils are configured. While much of the dendritic structure is annealed away during heat treatment, the homogenization is never complete and studies show that internal stresses develop at

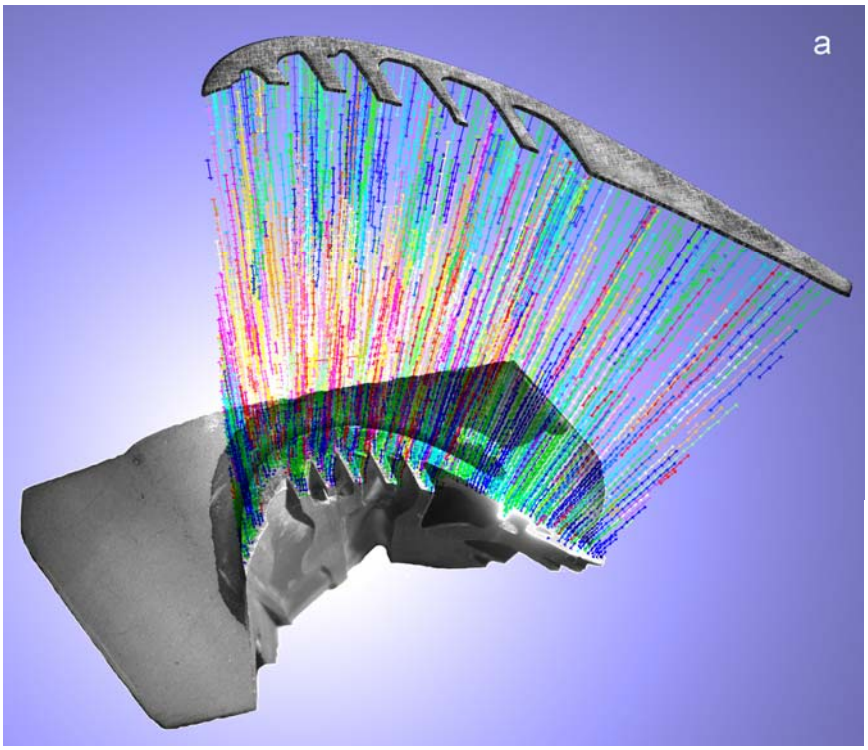

Figure 6: (a) Dendritic microstructure representation for a cast single crystal Ni-base superalloy turbine blade produced from serial sectioning and optical metallography. Colored lines map dendrite cores from base to top. Top of figure shows a metallographic section revealing dendrite cores. Note that blade has been 'filet' cut to reveal dendrite core locations relative to cooling channels of the airfoil. (b) Backscatter electron image of blade cross section showing crystal orientation contrast associated with low angle mis-oriented grains. (c) Optical micrograph of etched cross section showing dendrites and white eutectic particles. (d) Backscattered electron images of etched cross section showing the finer microconstituents of a typical superalloy blade. Images

the scale of the dendrite spacing (Epishin et al. 2004). Pore and eutectic microconstituents (including carbides) tend to be locally soft or hard relative to the

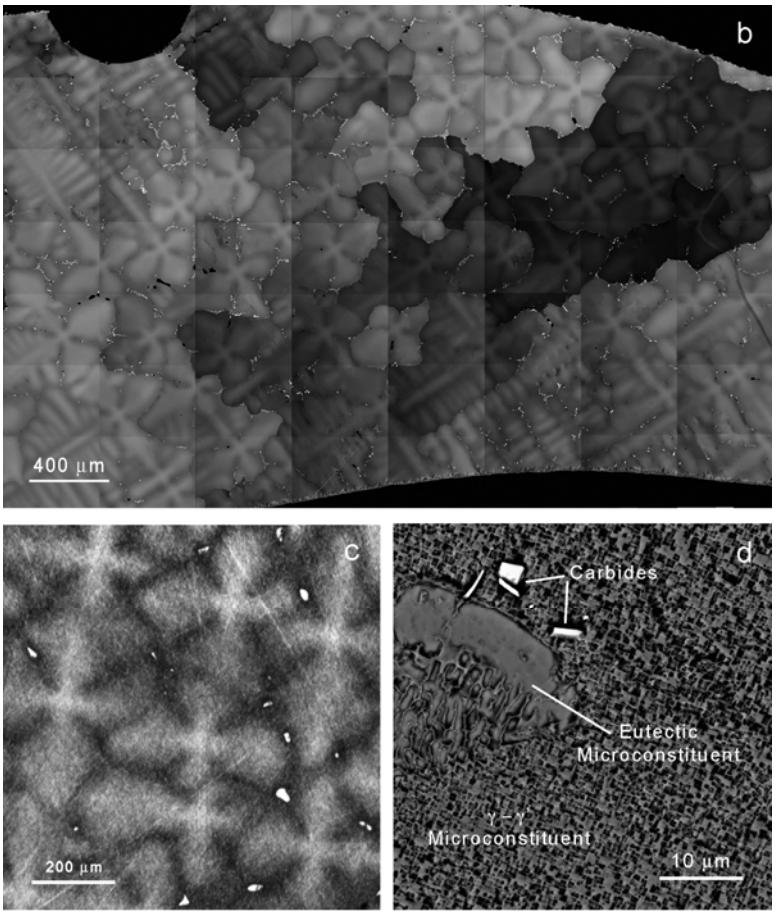

Figure 6: Continued.

matrix, thus concentrating strain under load and leading to fatigue crack initiation (Yi et al. 2007, Liu et al. 2008). Thus, each of these features affect internal stresses but is not taken into account within current design methods. In fact, even when design practice extends beyond treatments of the single-crystal superalloy materials as elastic solids, these microstructural features are not directly included.

4.2.2 Deficiencies in the Processing–Properties–Design Paradigm

The standard practice for including creep or fatigue response into a design falls back on the previously described processing–properties-design paradigm for materials engineering. The material is represented by a database of design minima curves from testing and basic feature configurations derived from experience. Non-destructive inspection methods are used to assure that cast blade crystal orientations are within the bounds set by the design curves and to selectively inspect for other defects. To establish those limitations, one might produce cast bars (having net sections much larger than the airfoils themselves) from which test specimens are prepared to evaluate creep and fatigue properties at a macroscopic scale. While a single primary crystallographic orientation and the primary dendrite spacing may be evaluated for those bars, efforts rarely track/control other aspects of microstructure. Thus, the processing–properties–design paradigm employed in this case implicitly assumes that: i) the cast microstructure of those specimens represents the same microstructures found in the turbine blade configurations, ii) the stochastic variations of properties within populations of tested specimens encompasses the property variations occurring within turbine blades and, iii) perhaps most importantly, that each of the microstructural details controlling properties is a homogeneous or equal-likelihood-of-occurrence entity over the configuration of the turbine blade. Within this paradigm, the "local continuum" (local) approximation is implicitly invoked well above the scale of key microstructural features, simply by the choice of specimens and scales used for determining material behavior.

Nowhere within the processing–properties–design paradigm does one explicitly consider the correlation lengths (de-correlation lengths) for the stochastic variations of microstructural features, even though the local approximation cannot hold below such correlation lengths. Further, nowhere during these procedures, except perhaps by de-rating material performance capability (design minima) does one tailor the design process for the fact that some microstructure attributes cannot be homogenized. As examples, at the scale of the turbine blade feature sizes, freckle defects and low angle grain structures occur having only one to three features through the wall thickness. These are not present in sufficient numbers to be statistically or homogeneously represented over the airfoil. Coarse features such as these do not have a correlation length within the context of the turbine blade and, may not have one even at the larger scale of the tested specimens.

The notion of establishing the de-correlation length for controlling microstructural features is an important one for setting foundations of microstructure–property relationship simulations. That notion is pervasive and may lead to better foundations from which to build quantitative MSE tools and techniques. For example, chapters of

this book suggest that fundamental scientific questions remain open regarding the viability of establishing representative volume elements (RVE) for evolving path-dependent plastic properties (for example see Choi and Brockman Chapter 6, Bronkhorst et al Chapter 7). At the scale of dislocations and substructure evolution, no quantitative theory exists and empirical approaches have not developed much beyond the scalar 'dislocation density' and associated hypotheses. At the scales of grain structure, basic questions centered on establishing the correlation length for grain-grain interaction effects in a 3d elastic-viscoplastic zone or for 3d plastic front propagation, remain relatively unaddressed except for highly idealized cases (Choi and Brockman Chapter 6, Simonovski et al. 2004). From a multiscale science and physics perspective such absences make the prospects for accurate predictive simulations of failure properties, such as crack initiation, rather remote since the kinematical driving forces would not be known even if the atomic processes could be adequately represented. For such properties, one engineering challenge is to establish a protocol, using accessible methods for microstructure RVE construction, to assess the validity and inaccuracies of property simulations. Consequently, aspects of material property variability and design minima are perhaps reflections of the under-developed materials–design interface in that there are no sufficient methods to treat unsolved materials science issues within engineering design. These may also illustrate a growth area needed within microstructure–properties based materials engineering and computational methods for microstructure–property relationship.

4.2.3 A Look Forward

Current research is exploring the use of concepts developed by Ghosh, et al. (2001, 2007, 2008, Swaminathan et al. 2006a, 2006b), for 2d simulations of long-fiber composites, to build a framework for microstructure–property–design simulations of turbine blades (Groeber 2009). At the scale of the entire blade, many analysis iterations are needed and a substantial number of volumetric analysis nodes are demanded simply from the spatial variation and complexity of the blade features. Therefore the structure representations and analysis methods must be computationally quick or fast acting.

Following Figures 5 and 6, there are at least four steps to representing turbine airfoils at this scale. First, one needs to define a structure representation having sufficient fidelity to represent both the engineering design geometry and the microstructural features too large or heterogeneous to be represented within a single local continuum entity. One may also chose to represent distinct defect structures as identifiable features at this scale. Second, validated constitutive descriptions are

needed for the property response of selected interest. These flow rules are assigned to the discrete continua of the structure representation. However, a key open aspect of these flow rules is the level of finer-scale microstructure and/or failure criteria that they represent (MacLachlan et al. 2001, Harrison et al. 2004, Ma et al. 2008, Choi et al. 2009). Usually, an anisotropic elastic-viscoplastic yield function or state-variable model, with or without crystallography and/or a damage model, would be the highest level of complexity that could be carried at this scale. Third, steps one and two need to be established within a numerical framework that is self-consistent with those selections. Within Ghosh's scheme, a concurrent adaptive finite element method is preferred since such methods permit natural strain or damage localization during the strain evolution and couples them to lower length-scale aspects of the microstructure. Finally, a formal engineering protocol requires that a parameterization and validation testing methodology be established at the same dimensional scale as the microstructural discreteness selected for the blade representation. For this example, that engineering requirement implies isolating, sectioning and testing various feature and specimen sizes from actual airfoils, rather than from separate test bars as current procedures employ.

The first three steps just described constitute an adaptation of what is termed a "Level 0" (L0) or part domain analysis within Ghosh's scheme. However, one still needs to rigorously tie these to lower scale microstructural features and micromechanisms of behavior as deformation and damage evolve during analysis. To achieve this, Ghosh's method defines a "Level 1" (L1) analysis domain at lower scale, for two reasons. Within the L1 domain a statistically equivalent representative volume element (SERVE) may be defined from microstructure characterization and descriptor set development coupled with standard asymptotic homogenization methods (Swaminathan et al. 2006a, 2006b). These SERVEs are used to numerically compute the anisotropic yield functions used for L0 analysis and may be iterated to include the intrinsic statistical variations of microstructure. In addition, as a L0 domain simulation run evolves, the coupling of far-field loads to geometric and coarse microstructural features begins to localize against pre-selected criteria. The concurrent adaptive numerical scheme permits a new L1 SERVE analysis domain to be inserted, as a periodic domain that introduces a higher level of microstructural fidelity that interacts with the now localizing (stress) fields. Methods for establishing these domains and selected criteria for tracking localization have been previously described and are treated within Chapter 4 of this work (Valiveti and Ghosh 2007, Chapter 4).

For turbine blade analysis, establishing the L1 analysis tools presents several challenges. By definition, the L1 representation can only comprise microstructural features whose correlation length is smaller than the SERVE for that domain. That is, the microstructural features must be amenable to computational homogenization at

that scale. In this example, low angle grain structures and freckle grains would not qualify; however, the dendritic structure may.

Characterization methods are needed for the dendritic microstructure to ascertain how many dendrite features are sufficient to establish the internal dendritic stress state. As Figure 7 shows, Shade (2008) has made some progress in this regard by showing that differences in flow stress between dendrite cores and interdendritic regions can be directly measured. Also, the L1 representation must carry most aspects of the γ–γ' microconstituent and any variations of it that may occur at the scale of the dendrites. What remains unclear in this example of the L1 domain is how much of the interdendritic microconstituents (eutectics, carbides and pores) can be or should be represented at the L1 scale. Hence, a challenge for the materials engineer developing

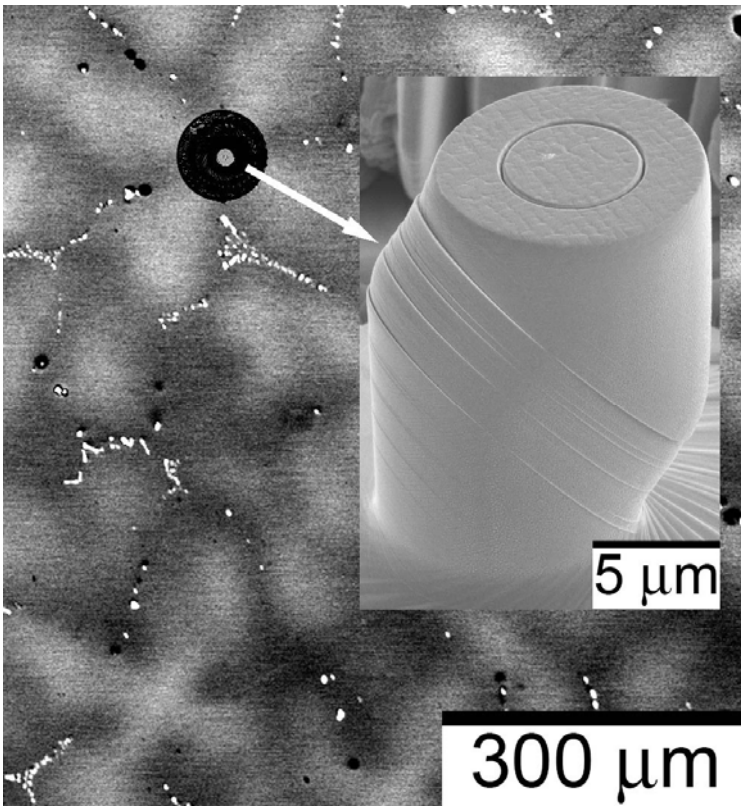

Figure 7: Microcrystal compression sample machined from dendrite core structure of cast single crystal superalloy and tested (Shade 2008).

computational methods for microstructure–property relationships is to establish both the microstructural de-correlation lengths, testing methods that correspond to those lengths and rigorous statistical representations of the microstructure variability.

As Ghosh, et al., describe, a quantitative partitioning of the computational domain will inevitably lead to identifiable microstructural features that cannot or should not be homogenized within a selected L1 domain (Ghosh Chapter 4). For the turbine blade example one may anticipate that the eutectic microconstituent or pores that exceed some size dimension would fall into that realm. These are defined as Level 2 (L2) features. Any such features need to be represented within their own micromechanics frameworks that account for plastic processes and damage accumulation within those entities. Even coarse-scale extrinsic defects may fall into a similar L2 domain since they cannot be homogenized via asymptotics. For the intrinsic microstructural variation, as simulations proceed at the L0 and L1 levels, again localization is expected that will exceed the bounds of pre-selected failure criteria established within failure or damage models. Once that occurs, the adaptive scheme inserts a L2 domain into localization fields and permits a still higher fidelity representation of behavior to evolve in simulations. For the turbine blade material example one may envisage that L2 computational methods consist of crystal plasticity models, non-local formulations of damage, or crack initiation models of various forms. Clearly the concurrent multiscale adaptive scheme described here can be explicitly tied to microstructural–dependent properties and heterogeneous materials, to the extent that its various parts can be build in a computationally viable way.

4.3 Advanced Engineering Design – a Virtual Materials Systems Paradigm

Previously the notion of virtual materials systems was introduced as a parallel to virtual biological systems. One may expect that as virtual materials systems become closer to reality, so too will the interface between design engineering and MSE further dissolve. Figure 4 described what is becoming current-day practice within the ICME paradigm for materials, which already contains broad overlap between design and materials. Here, that view is contrasted with a futuristic view partially described in previous reports (Dimiduk et al. 2004a, Dimiduk 2004b). The view outlined the potential of virtual materials systems or virtual processing–microstructure–property–design relationships to affect the engineering design practices, especially for developing an unknown. Figure 8 describes a design environment wherein the usual suite of engineering tools for shape and product performance in a mechanical engineering sense (boxes A and B), are integrally coupled to a comparable suite of

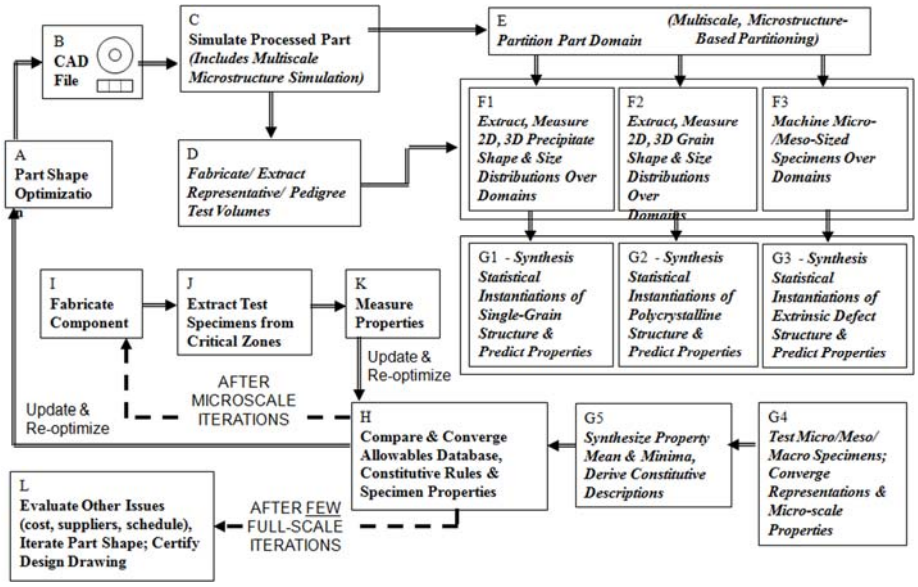

Figure 8: Schematic depiction of the microstructure–property aspects of the virtual materials systems paradigm. This paradigm places significant emphasis on building and using a validated representation of the material, via a suite of integrated small-scale experimental and simulation methodologies, as an integral part of the system design process. Within such an approach, there are no real boundaries between engineering design and materials engineering.

design tools for microstructure–property relationships. Boxes E, F, and G describe microstructure sensitive representations of the part. From this one may synthesize probability of part population behavior, then link these to system fleet probability of behavior via other probabilistic tools.

One may envisage an environment (Figure 8) for which process modeling includes spatial-temporal simulations of microstructure evolution, at both the level of primary constituent kinematics (grain, fiber or primary matrix constituent level) and at the lower levels of microconstituent and defect chemical and kinetics behavior (box C). Utilizing those tools results in a virtual description of the part domain. The figure shows that the process modeling procedures result in two key attributes for the remaining design system. First, as suggested by box D, experiments would be initiated that are defined from the results of process simulations and are specifically

focused on evaluating critical microstructures or pedigreed materials for bounding models.

In parallel to the experimental activity, box E suggests that the preliminary designed part may be partitioned into microstructural simulation domains. These can be defined from the both the spatial-temporal variations of continuum state-variable fields and from expectations of extrinsic defect influences on behavior. For each of those domains, SERVE must be constructed to manage the intrinsic evolution of both the grain or primary-constituent kinematics, as well as the lower-scale, single-grain or microconstituent level kinetics under service loads and environmental conditions. Construction of the RVE suite involves both small-scale experimental measurements and a more-substantial set of simulation-based activities that includes building synthetic statistical instantiations of microstructures that include imposed extrinsic defect structures. Those activities are shown in boxes F1-G4 in Figure 8. The activities depicted in box G5 represent the use of the small scale SERVE suite within simulation frameworks that derive a statistically-relevant set of material responses, to include probabilities of performance. These result in larger-scale constitutive descriptions with damage mechanisms and 'materials allowables' for part design. The synthetically derived materials behavior descriptions are then reconciled and adjusted using information from historical databases for similar material behavior (box H).

From this point the whole set of procedures may be iterated and updated toward some optimization criteria, until there is a converged quantitative view of the expected microstructure–property relationships over all domains of a part, consistent with the desired design performance criteria. Only after such reconciliation of design goals would one have to prepare full-scale test articles for full certification of the part. Clearly, within such a future paradigm, there is little separation between MSE and design engineering. For such a paradigm, "design with materials" becomes symbiotically fused with "design of materials." This is done in such a way that simulated responses are fused with heuristically known responses resulting in both cost and performance risk reductions.

For such a long-term view of microstructure–property–design engineering as depicted in Figure 8 to become a reality, it is important that virtual materials systems build from technologies that are viable today, but remain extensible into the representations of tomorrow. As previously discussed, one area that already poses a present-day challenge, for which today's decisions will impact the broader longer-term evolution of the field, is data types and management. For example, the last five years have seen step-wise growth in the techniques for both characterizing microstructures in 3d and simulating their behavior. Those successes brought about what some have a called a 'data tsunami.' Both models and experiments now overwhelm data management, storage and, most importantly analysis capabilities. The very existence of such data, together with the interests in mining such data, calls for extensible data

structures that carry the data pedigree throughout and, for automated, unsupervised analysis tools especially for microstructural analysis.

5 The Present Book

No book on microstructure–property sciences and techniques can be comprehensive, nor was it the goal of the editors of this work to cover the topic in a comprehensive way. Rather, the purpose of this book is to provide insights into selected aspects of microstructure–property science and provide views of what is in the realm of the possible when a computation and simulation centric perspective is adopted. By doing this, the editors believe that a vision for the future of the field can be shown, specific advances in the field conveyed and, gaps in the computational methods highlighted.

The structure of the book follows to great degree from the introductory context discussed previously. The view is that the broad goal of attaining virtual materials systems provides the guiding principles and, that the four domains of multiscale materials modeling (Figure 5) together with microstructure–property science provide the more detailed structure. Thus, the book consists of four parts. Part I describes selected methods for attaining virtual materials structure and directly tying that information to the computational domain, beginning with methods for experimentally determining 3d microstructure. Following that, techniques for representing grain structure information in descriptor form are described together with methods to apply computational techniques with those descriptors to generate statistically equivalent microstructures. The last two chapters of Part I describe how microstructural information should be directly used to establish representative volume elements for simulations and, the state of the art in microstructure evolution or kinetics modeling and how those techniques couple to experimental data.

Part II of the book shifts the focus onto virtual material response within the simulation environment, which is directly tied to the constitutive descriptions selected for simulation. There is a chapter that discusses the readiness of present-day finite element method codes for treating microstructure–property relationships. That subject gains importance as one realizes that today's methods are principally developed for stress analysis of engineering structures or metal deformation processing, not for micromechanical behavior of heterogeneous anisotropic materials. The second chapter on materials response treats constitutive equations for microstructural effects in metal forming and illustrates what a challenge the topic brings. The following chapter treats a non-local method for establishing a length-scale dependent kinematical description (aspects of size effects) for materials simulation. Finally, Part II concludes

with a discussion of time-dependent material behavior and the challenges of treating that in the simulation domains.

In Part III the book describes selected numerical techniques and simulation frameworks for treating aspects of engineering challenges. There is a description of material point models that have been tied to texture analysis of materials for some time and, a chapter on a full-field spectral method for viscoplastic deformation analysis. Part III also includes a chapter that describes error, stability and limits to homogenization within numerical techniques. Since most of the driving force for microstructure–property analysis stems from a need to understand probabilistic cracking behavior of structures, there is a chapter that specifically describes the state-of-the-art in that field. Finally, Part III concludes with a description of a completely new multiscale method for the time domain. This method may permit analysis of certain fatigue problems with a highly reduced demand for computational capacity.

While the first three parts of this work develop many key aspects of microstructure–property science from a computational perspective, there is still a great deal missing. Within Part IV of the book three selected and current broader-interest topics in the MSE community are presented. This part includes a chapter on the use of parametric dislocation dynamics to elucidate basic strengthening behavior and stress fields below the grain level. Also, it includes a chapter that describes the multiscale framework for mechanical behavior testing that is evolving in parallel to the ICME paradigm. The final chapter returns to a broader look at the design and MSE fields and provides another perspective on the challenges of bringing microstructure–property information into the systems engineering optimization domain.

The editors of this work operate from the strong belief that there is a quiet revolution under way within microstructure–property science that is being driven by the continuing advances in computing capabilities. That revolution is allowing designers to explicitly include microstructure heterogeneity and location- or feature-specific behavior directly within the design process. Ultimately this revolution will lead to the availability of virtual materials systems and hopefully to portable materials that are no longer so closely tied to application-specific processes and descriptions. While much of this book describes the advances from the perspectives of metals technologies, there is ample reason to believe that the structuring of the challenges and aspects of the techniques are general and applicable to broad classes of materials beyond metals. Nonetheless, even for metals many of the techniques require significant further developments to realize engineering gains. Our hope is that many will be swayed by the art of the desirable that is conveyed herein and find ways to transform that into the art of the possible while continuing to advance the field.

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